

10/607,220

* * * * * STN Columbus * * * * *

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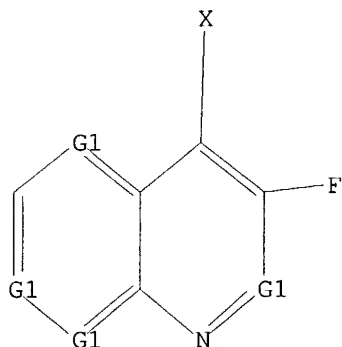
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L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 C,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

L3 39 SEA SSS FUL L1

=> file ca

=> s l3

L4 40 L3

=> s l3/prep

40 L3

3150725 PREP/RL

L5 22 L3/PREP

(L3 (L) PREP/RL)

=> d ibib abs fhitstr 1-22

L5 ANSWER 1 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 137:24717 CA
 TITLE: Preparation of 4-piperazinoquinolines which inhibit phosphorylation of a PDGF receptor
 INVENTOR(S): Scaenough, Robert M.; Pandey, Anjali
 PATENT ASSIGNEE(S): Millennium Pharmaceuticals, Inc., USA
 SOURCE: PCT Int. Appl., 151 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002072578	A2	20020919	WO 2002-US7187	20020308
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 2003004158	A1	20030102	US 2002-94191	20020308
PRIORITY APPLN. INFO.:			US 2001-273951P	P 20010308
OTHER SOURCE(S):		MARPAT 137:24717		

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I: V = O, S, N(CN); W = (un)substituted 1,4-piperazinediyl, 1,4-homopiperazinediyl; X = H, Tz, F, Cl; Z = OH, CN, CHO; T = ci-16 alkylidene optionally interrupted by O, S, CO₂, OCO, CO;

R1 = H, (un)substituted C1-16 alkyl, C2-16 alkenyl, etc.; R2 = H, (un)substituted C1-16 alkyl, C2-16 alkenyl, etc.; R3-R6 = H, halo, alkyl, etc.] which inhibit phosphorylation of a PDGF receptor to hinder abnormal cell growth and cell wandering, and a method for preventing or treating cell-proliferative diseases such as arteriosclerosis, vascular reobstruction, cancer and glomerulosclerosis, were prepd. Thus, reacting 4-chloro-6-methoxy-7-(3-piperidylpropoxy)quinoline-3-carbonitrile (prepn. given) with N-(4-isopropoxyphenyl)piperazinecarboxamide hydrochloride in the presence of K₂CO₃ in DMF afforded 69% II which showed IC₅₀ of 0.134 .mu.M and 0.060 .mu.M in M63 w/human plasma phosphorylation assay and in HR5 phosphorylation assay, resp.

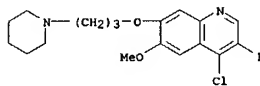
IT 460088-42-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of 4-piperazinoquinolines which inhibit phosphorylation of a PDGF receptor)

RN 460088-42-0 CA

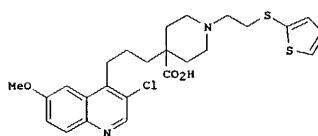
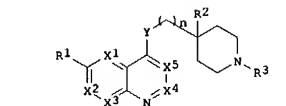
L5 ANSWER 2 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 136:386033 CA
 TITLE: Heterocyclylalkyl piperidine derivatives, particularly
 4-[3-(quinolin-4-yl)propyl]piperidine-4-carboxylic acids, their preparation and compositions containing same, for use as antibacterials.
 INVENTOR(S): Bacque, Eric; Carry, Jean-Christophe; El-Ahmad, Youssef; Evers, Michel; Hubert, Philippe; Malleron, Jean-Luc; Mignani, Serge; Pantel, Guy; Tabart, Michel;
 PATENT ASSIGNEE(S): Viviani, Fabrice
 SOURCE: Aventis Pharma S.A., Fr.
 PCT Int. Appl., 362 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002040474	A2	20020523	WO 2001-FR3559	20011114
WO 2002040474	A3	20021031		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
FR 2816618	A1	20020517	FR 2000-14738	20001115
FR 2816618	B1	20021227		
AU 2002018365	A5	20020527	AU 2002-18365	20011114
US 2002111492	A1	20020815	US 2001-987386	20011114
US 6603005	B2	20030805		
EE 200300207	A	20030815	EE 2003-207	20011114
EP 1337529	A2	20030827	EP 2001-996538	20011114
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, EL, TR			
BR 2001015312	A	20030923	BR 2001-15312	20011114
JP 2004514661	T2	20040520	JP 2002-543484	20011114
NO 2003002187	A	20030626	NO 2003-2187	20030514
PRIORITY APPLN. INFO.:			FR 2000-14738	A 20001115
			US 2000-255145P	P 20001214
			WO 2001-FR3559	W 20011114
OTHER SOURCE(S):		MARPAT 136:386033		

L5 ANSWER 1 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)
 CN Quinoline, 4-chloro-3-fluoro-6-methoxy-7-[3-(1-piperidyl)propoxy]-
 (9CI)
 (CA INDEX NAME)



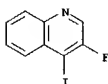
L5 ANSWER 2 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)



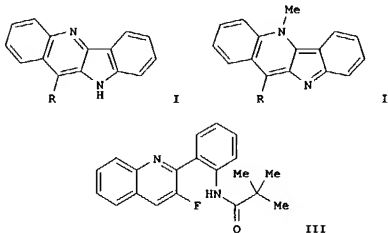
AB The invention concerns heterocyclylalkyl piperidine deriva. I, including their enantiomeric or diastereoisomeric forms, or mixts. thereof, and/or their syn or anti forms, or mixts. thereof, and their salts [wherein X1, X2, X3, X4, and X5 = C(R'1), C(R'2), C(R'3), C(R'4), C(R'5), or one of X-groups (at most) = N; R1, R'1, R'2, R'3, R'4, R'5 = H, halo, alkyl, cycloalkyl, Ph, PhS, OH, heterocyclyl, cyano, CO₂H, alkoxy, carbonyl, (un)substituted NH₂, etc.; R2 = CO₂H, alkoxy, carbonyl, cycloalkoxy, carbonyl, cyano, CONR₂Ar, CH₂OH, substituted alkyl, CF₂-Rc, C(CH₃)₂-Rc, CORc, CH(OH)-Rc, C(cycloalkyl)-Rc, or CH:CH-Rc; Ra, Rb = H, alkyl, cycloalkyl, Ph, heterocyclyl; or NR₂Ar = (un)substituted 5- or 6-membered heterocycle; Rc = CO₂H, alkoxy, carbonyl, cycloalkoxy, carbonyl, CONR₂Ar; R3 = Ph, heterocyclyl, various substituted alkyls; Y = CH(Re), CF₂, C(:NOH), alkoxy, iminomethylene, cycloalkoxy, iminomethylene, or C3-6 cycloalkylidene; Re = H, F, OH, alkoxy, cycloalkoxy, CO₂H, alkoxy, carbonyl, NR₂Ar, CONR₂Ar; and n = 0-4; wherein the radicals or Ph or heterocyclyl portions mentioned above can optionally be substituted]. Approx. 60 compds. were prepd., 5 were specifically claimed, and many more names were listed. For instance, Pd-complex-catalyzed coupling of 4-allyl-4-Cbz-1-BOC-piperidine with 4-bromo-3-chloro-6-methoxyquinoline (prepn. of both compds. given), followed by removal of the BOC group with CF₃CO₂H, N-alkylation with 2-[(2-bromoethyl)thio]thiophene, and hydrolysis of the benzyl ester (Cbz) in aq. HCl, gave title compd. II as the di-HCl salt. I are active against both gram-pos. and gram-neg. bacteria. I were active against exptl. infection of mice with Staphylococcus aureus IP8203 at 18-150 mg/kg s.c., or 20-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c. (2 administrations).

IT 213772-63-SP, 3-Fluoro-4-iodoquinoline
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP

L5 ANSWER 2 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)
 (Preparation); RACT (Reactant or reagent)
 (intermediate; prepn. of quinolinylpropylpiperidinecarboxylic acids as
 antibacterials.)
 RN 213772-63-5 CA
 CN Quinoline, 3-fluoro-4-iodo- (9CI) (CA INDEX NAME)

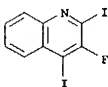


L5 ANSWER 3 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 134:295759 CA
 TITLE: New synthesis of benzo-.delta.-carbolines,
 cryptolepines, and their salts: in vitro cytotoxic,
 antiparasitic, and antitrypanosomal activities of
 delta.-carbolines, benzo-.delta.-carbolines, and
 cryptolepines
 AUTHOR(S): Arzel, Erwan; Rocca, Patrick; Grellier, Philippe;
 Labaie, Mehdi; Frappier, Francois; Gueritte,
 Francoise; Gaspard, Christiane; Marsais, Francis;
 Godard, Alain; Queguiner, Guy
 CORPORATE SOURCE: UMR 6014, Institut National des Sciences Appliquees,
 Mont-Saint-Aignan, 76131, Fr.
 SOURCE: Journal of Medicinal Chemistry (2001) 44(6), 949-960
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:295759
 GI



AB Benzo-.delta.-carbolines I and cryptolepines II (R = H, Me, Et, Pr, Ph)
 and their salts were prepd. using strategies based on the assocn. between
 halogen-dance and hetero-ring cross-coupling. The syntheses are fully
 convergent and regioselective with overall yields of 27-70%. Thus,
 coupling of 3-fluoro-2-iodoquinoline with the phenylboronate
 2-(Me3CONH)C6H4(OH)2 gave the phenylquinoline III. Treatment of III
 with pyridinium chloride at 215.degree. for 30 min and then with aq. NH3
 gave 83% I (R = H). A halogen-dance mechanism in the quinoline series
 was proposed. The formal synthesis of potential antimalarial compds. and the
 first total synthesis of 11-isopropylcryptolepine was described.
 Cytotoxic activity against mammalian cells and activities against
 Plasmodium falciparum and Trypanosoma cruzi of benzo-.delta.-carbolines
 and .delta.-carbolines were evaluated in vitro to study the

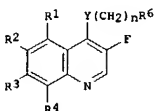
L5 ANSWER 3 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)
 structure-activity relationships. For benzo-.delta.-carbolines,
 methylation at N-5 increases the cytotoxic and antiparasitic activities.
 A further alkylation on C-11 generally increases the cytotoxic activity
 but not the antiparasitic activity, cryptolepine and
 11-methylcryptolepine
 being the most active on both parasites. Taking advantage of the
 fluorescence of the indoloquinoline chromophore, cryptolepine was
 localized by fluorescence microscopy in parasite DNA-contg. structures
 suggesting that these compds. act through interaction with parasite DNA
 as proposed for cryptolepine on melanoma cells. For .delta.-carbolines,
 methylation at N-1 is essential for the antimalarial activity.
 1-Methyl-.delta.-carboline specifically accumulates in the intracellular
 parasite. It has weak cytotoxic activity and can be considered as a
 potential antimalarial compd.
 IT 213772-72-6V
 RL: RCT (Reactant); PREP (Preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (cytotoxicity and antiparasitic/antitrypanosomal activities of
 benzo-.delta.-carbolines and cryptolepines prepd. via regioselective
 cross-coupling reactions)
 RN 213772-72-6 CA
 CN Quinoline, 3-fluoro-2,4-diiodo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR
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 RECORD. ALL CITATIONS AVAILABLE IN THE RE
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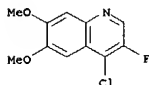
L5 ANSWER 4 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 133:350151 CA
 TITLE: Preparation of quinoline derivatives as inhibitors of
 MEK enzymes
 INVENTOR(S): Gibson, Keith Hopkinson
 PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
 SOURCE: PCT Int. Appl., 51 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000068199	A1	20001116	WO 2000-GB1698	20000503
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
BR 2000010366	A	20020213	BR 2000-10366	20000503
EP 1178965	A1	20020213	EP 2000-927492	20000503
EP 1178965	B1	20030924		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
TR 200103185	T2	20020521	TR 2001-200103185	20000503
AT 250582	E	20031015	AT 2000-927492	20000503
US 6638945	B1	20031028	US 2001-959434	20011025
ZA 2001008969	A	20030130	ZA 2001-8969	20011030
NO 2001005447	A	20011212	NO 2001-5447	20011107
PRIORITY APPL. INFO.:			GB 1999-10580	A 19990508
OTHER SOURCE(S):		MARPAT 133:350151	WO 2000-GB1698	W 20000503
GI				



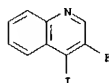
AB The title compds. I [n = 0-1; Y = NH, O, S, NR7 where R7 is alkyl of 1-6
 carbon atoms; R6 = cycloalkyl, pyridinyl, pyrimidinyl, Ph; or R6 is a
 group R8XR9 and X is selected from CH2, NH, O, S, NR5; R1, R2, R3, R4 =
 H,
 OH, halo, cyano, NO2, etc.], inhibitors of MEK enzymes, were prepd.
 E.g.,

L5 ANSWER 4 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)
 reaction of 4-chloro-6,7-dimethoxy-3-fluoroquinoline (prepn. given) and
 4-(2-methoxyphenoxy)aniline gave
 4-(2-methoxyphenoxy)anilino-3-fluoro-6,7-
 dimethoxyquinoline.
 IT 205448-48-22
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**
 (Preparation); RACT (Reactant or reagent)
 (prepn. of quinoline deriva. as inhibitors of MEK enzymes)
 RN 205448-48-2 CA
 CN Quinoline, 4-chloro-3-fluoro-6,7-dimethoxy- (9CI) (CA INDEX NAME)



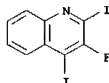
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
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L5 ANSWER 5 OF 22 CA COPYRIGHT 2004 ACS on STN
 132:3495 CA
 TITLE: First total synthesis of cryptomisine
 AUTHOR(S): Arzel, Erwan; Rocca, Patrick; Marsais, Francis;
 Godard, Alain; Queguiner, Guy
 CORPORATE SOURCE: UPRES-A 6014 - IRCOF/INSA de Rouen, Mont Saint
 Aignan, 76131, Fr.
 SOURCE: Tetrahedron (1999), 55(41), 12149-12156
 CODEN: TETRA; ISSN: 0040-4020
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 132:3495
 AB The first total synthesis of cryptomisine, a novel
 indolo[3,2-b]quinoline
 dimeric alkaloid from *Cryptolepis sanguinolenta*, is reported. The
 approach is based on a convergent methodol. which involves a new
 halogen-dance reaction in 3-fluoro-4-iodoquinoline followed by its
 cross-coupling reaction to give bis-2-iodo-3-fluoroquinolin-4-ylmethanol
 which couples with 2-pivaloylaminoxyphenylboronic acid and then
 heterocyclizes to cryptomisine.
 IT 213772-63-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**
 (Preparation); RACT (Reactant or reagent)
 (total synthesis of cryptomisine)
 RN 213772-63-5 CA
 CN Quinoline, 3-fluoro-4-iodo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR
 THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
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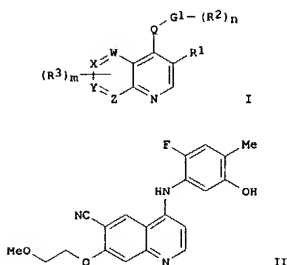
L5 ANSWER 6 OF 22 CA COPYRIGHT 2004 ACS on STN
 129:276078 CA
 TITLE: First halogen-dance reaction in quinoline series:
 application to a new synthesis of quindoline
 AUTHOR(S): Arzel, Erwan; Rocca, Patrick; Marsais, Francis;
 Godard, Alain; Queguiner, Guy
 CORPORATE SOURCE: UPRESA 6014 CNRS - IRCOF/INSA de Rouen, Mont Saint
 Aignan, 76131, Fr.
 SOURCE: Tetrahedron Letters (1998), 39(36), 6465-6466
 CODEN: TETRA; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 129:276078
 AB The first halogen-dance reaction in the quinoline series is described and
 was applied to a new convergent synthesis of quindoline, a natural
 benzo-.delta.-carboline.
 IT 213772-72-6P
 RL: SPN (Synthetic preparation); **PREP** (Preparation)
 (halogen-dance reaction in quinolines)
 RN 213772-72-6 CA
 CN Quinoline, 3-fluoro-2,4-diiodo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR
 THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L5 ANSWER 7 OF 22 CA COPYRIGHT 2004 ACS on STN
 128:270546 CA
 TITLE: Quinoline derivatives inhibiting the effect of growth
 factors such as VEGF
 INVENTOR(S): Thomas, Andrew Peter; Hennequin, Laurent Francois
 Andre; Ple, Patrick Alan
 PATENT ASSIGNEE(S): Zeneca Ltd., UK; Zeneca Pharma S.A.; Thomas, Andrew
 Peter; Hennequin, Laurent Francois Andre; Ple,
 Patrick
 SOURCE: Alan
 PCT Int. Appl., 129 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9813350	A1	19980402	WO 1997-GB2587	19970923
W:	AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GB, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
AU 9743137	A1	19980417	AU 1997-43137	19970923
AU 733551	B2	20010517		
EP 929526	A1	19990721	EP 1997-941115	19970923
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI			
CN 1237963	A	19991208	CN 1997-199929	19970923
JP 2001500890	T2	20010123	JP 1998-515386	19970923
NO 9901423	A	19990511	NO 1999-1423	19990324
KR 2000048575	A	20000725	KR 1999-702502	19990324
PRIORITY APPLN. INFO.:			EP 1996-402034	A 19960925
			WO 1997-GB2587	W 19970923
OTHER SOURCE(S):			MARPAT 128:270546	
GI				



AB The invention relates to the use of compds. I [R1 = F or H; R2 = OH, halo, C1-3 alkyl, C1-3 alkoxy, C1-3 alkanoyloxy, CF3, cyano, amino, or NO2; n = 0-5; Q = O, NH, S, or CH2; G1 = Ph or 5- to 10-membered heteroarom. cyclic or bicyclic contg. O, S, and/or N; W, X, Y, Z = CH or N (but all 4 .noteq. N); m = 1-3; R3 = H, OH, halo, cyano, NO2, CF3, C1-3 alkyl, NR4R5 (wherein R4 and R5 = H or C1-3 alkyl), or R6X1- wherein X1 = CH2 or heteroatom linker group, and R6 = alkyl, alkenyl or alkynyl chain (un)substituted by OH, amino, NO2, alkyl, cycloalkyl, alkoxyalkyl, (un)substituted pyridone, Ph, heterocyclyl, etc. (which alkyl, alkenyl or alkynyl chain may have heteroatom linker), or R6 = (un)substituted pyridone, Ph, or heterocyclyl], and salts thereof, in the manuf. of medicaments for prodn. of an antiangiogenic and/or vascular permeability-reducing effect. Also disclosed are processes for the prepn. of I, and pharmaceutical compns. contg. them as active ingredients. I and salts inhibit the effects of VEGF, a property useful in the treatment of a no. of disease states including cancer and rheumatoid arthritis (no data). Examples include 63 syntheses and 7 general formulations. For instance, condensation of 4-chloro-6-cyano-7-(2-methoxyethoxy)quinoline hydrochloride with 2-fluoro-5-hydroxy-4-methylaniline (prepn. given) in refluxing iso-PrOH gave 68% title compd. II, isolated as the HCl salt.

IT 205448-48-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; prepn. of quinoline derivs. as growth factor inhibitors)

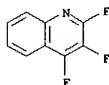
RN 205448-48-2 CA
 CN Quinoline, 4-chloro-3-fluoro-6,7-dimethoxy- (9CI) (CA INDEX NAME)

L5 ANSWER 8 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 127:346280 CA
 TITLE: Reactions of trifluorovinylolithium and 1-chloro-2,2-difluorovinylolithium: the synthesis of fluorinated heterocycles
 AUTHOR(S): Burdon, J.; Coe, P. L.; Haslock, I. B.; Powell, R. L.
 CORPORATE SOURCE: School of Chemistry, The University, Edgbaston, Birmingham, B15 2TT, UK
 SOURCE: Journal of Fluorine Chemistry (1997), 85(2), 151-153
 CODEN: JFLCAR; ISSN: 0022-1139
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Trifluorovinylolithium (from 1,1,1,2-tetrafluoroethane [HFC-134a]) reacted with 2-trifluoromethylaniline at -78 .degree.C to give 2,3,4-trifluoroquinoline in moderate to good yield. In a similar reaction, 1-chlorodifluorovinylolithium (from 1-chloro-2,2,2-trifluoroethane [HCFC-133a]) yielded 3-chloro-2,4-difluoroquinoline.

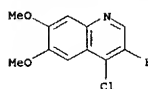
IT 198128-72-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of fluorinated heterocycles)

RN 198128-72-2 CA
 CN Quinoline, 2,3,4-trifluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

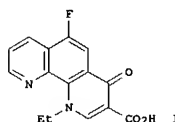


REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

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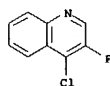
L5 ANSWER 9 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 122:133124 CA
 TITLE: Quinolone(II):synthesis of fluoro-substituted pyrido[3,2-h]quinolone derivatives as potential antibacterials
 AUTHOR(S): Lee, Jae Keun; Chang, Sha Joung
 CORPORATE SOURCE: Dep. Chem., Coll. Natl. Sci., Taegu, 702-701, S. Korea
 SOURCE: Korean Journal of Medicinal Chemistry (1994), 4(2), 92-100
 CODEN: KJMC7; ISSN: 1225-0058
 PUBLISHER: Korean Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English



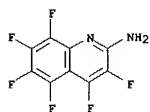
AB The potential antimicrobials, 1-ethyl-6-fluoro-1,4-dihydro-4-oxo-1,10-phenanthroline-3-carboxylic acid (I), 1-ethyl-1,4-dihydro-9-(4-methyl-1-piperazinyl)-4-oxo-1,10-phenanthroline-3-carboxylic acid and 1-ethyl-6-fluoro-1,4-dihydro-9-(4-methyl-1-piperazinyl)-4-oxo-1,10-phenanthroline-3-carboxylic acid were synthesized and their antibacterial activities were evaluated.

IT 161038-28-4P, 4-Chloro-3-fluoroquinoline
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of bactericides 4-oxo-1,10-phenanthroline-3-carboxylates)

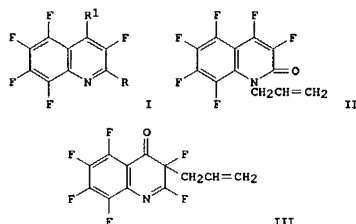
RN 161038-28-4 CA
 CN Quinoline, 4-chloro-3-fluoro- (9CI) (CA INDEX NAME)



L5 ANSWER 10 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 120:134243 CA
 TITLE: Remarkable orientational effects in the displacement of the fluorine from heptafluoroisoquinoline and -quinoline towards sulfur nucleophiles. Further reactions with oxygen nucleophiles
 AUTHOR(S): Brooke, Gerald M.; Chambers, Richard D.; Drury, Christopher J.; Bower, Michael J.
 CORPORATE SOURCE: Chem Dep., Sci. Lab., Durham, DH1 3LE, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1993), (18), 2201-9
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB 1,3,4,5,6,7,8-Heptafluoroisoquinoline (I) and 2,3,4,5,6,7,8-heptafluoroquinoline (II) have been treated with a variety of sulfur and oxygen nucleophiles and some reactivities have been measured relative to treatment with ethoxide. The significant feature is that the major sites of attack by the sulfur and the oxygen nucleophiles are significantly different: attack occurs at the 6-position by sulfur and the 1-position by oxygen nucleophiles in the isoquinoline deriv. I irresp. of the relative reactivities; and at the 4-position by sulfur and at both the 2- and 4-positions by oxygen nucleophiles in the quinoline deriv. II. The results have been rationalized on the basis of the relative hardness/softness of the nucleophiles and the known activating influences of the fluorine atoms at sites remote from the reaction center.
 IT 13180-57-9P
 RL: SPN (Synthetic preparation); **PREP** (Preparation) (prepn. of)
 RN 13180-57-9 CA
 CN 2-Quinolinamine, 3,4,5,6,7,8-hexafluoro- (9CI) (CA INDEX NAME)

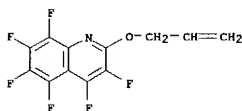


L5 ANSWER 11 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 110:38848 CA
 TITLE: The preparation and thermolysis reactions of allyl 3,4,5,6,7,8-hexafluoroquinolin-2-yl ether, allyl 2,3,5,6,7,8-hexafluoroquinolin-4-yl ether and allyl 3,4,5,6,7,8-hexafluoroisoquinolin-1-yl ether
 AUTHOR(S): Brooke, G. M.; Eggleston, I. M.; Hale, F. A.
 CORPORATE SOURCE: Chem. Dep., Sci. Lab., Durham, DH1 3LE, UK
 SOURCE: Journal of Fluorine Chemistry (1988), 38(3), 421-34
 CODEN: JFLCAR; ISSN: 0022-1139
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 110:38848
 GI

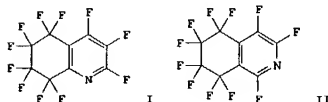


AB Reaction of $\text{CH}_2=\text{CHCH}_2\text{ONa}$ with 2,3,4,5,6,7,8-heptafluoroquinoline gave 67 and 20% of ethers I ($\text{R} = \text{CH}_2=\text{CHCH}_2$, $\text{R}_1 = \text{F}$; $\text{R} = \text{F}$, $\text{R}_1 = \text{CH}_2=\text{CHCH}_2$), resp. Thermolysis of I ($\text{R} = \text{CH}_2=\text{CHCH}_2$, $\text{R}_1 = \text{F}$) in tetralin at 212.degree. for 48 h gave 69% of the Claisen rearrangement product II in which N is the migration terminus. However, a similar rearrangement of I ($\text{R} = \text{F}$, $\text{R}_1 = \text{CH}_2=\text{CHCH}_2$) in o-xylene at 147.5.degree. for 2.5 h gave allylquinolinone III, the product with C as the migration terminus.
 IT 118097-74-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP** (Preparation); RACT (Reactant or reagent) (prepn. and Claisen rearrangement of)
 RN 118097-74-8 CA
 CN Quinoline, 3,4,5,6,7,8-hexafluoro-2-(2-propenyloxy)- (9CI) (CA INDEX NAME)

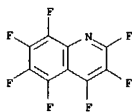
L5 ANSWER 11 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)



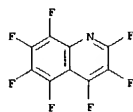
L5 ANSWER 12 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 107:23214 CA
 TITLE: Polyhalogenoheterocyclic compounds. Part 37. Perfluorotetrahydroquinoline, -isoquinoline, and related compounds
 AUTHOR(S): Bell, S. L.; Chambers, R. D.; Daniels, R.; Holmes, T. F.; Silvester, M. J.
 CORPORATE SOURCE: Dep. Chem., Univ. Sci. Lab., Durham, DH1 3LE, UK
 SOURCE: Journal of Fluorine Chemistry (1986), 32(4), 403-14
 CODEN: JFLCAR; ISSN: 0022-1139
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 107:23214
 GI



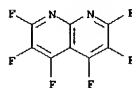
AB The formation of perfluorotetrahydroquinoline (I) and -isoquinoline II in the high temp. reaction between KF and heptachloroquinoline and -isoquinoline is investigated and a mechanism is proposed. I and II represent unusually substituted pyridine derivs. and the orientation of substitution in reactions with nucleophiles is reported.
 IT 13180-38-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); **PREP** (Preparation); RACT (Reactant or reagent) (prepn. and fluorination or chlorination of)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



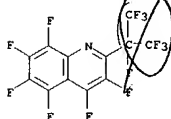
L5 ANSWER 13 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 84:135440 CA
 TITLE: Perfluorodicarboxylic acids, VI. Preparation of perfluoropyridine-2,3-dicarboxylic acid by oxidation of perfluoroquinoline
 AUTHOR(S): Sartori, P.; Ahlers, K.; Frohn, H. J.
 CORPORATE SOURCE: Fachber. Chem., Gesamthochsch. Duisburg, Duisburg, Fed. Rep. Ger.
 SOURCE: Journal of Fluorine Chemistry (1976), 7(4), 363-74
 CODEN: JFLCAR; ISSN: 0022-1139
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 AB The oxidn. of perfluoroquinoline with 98% HNO₃ yields perfluoropyridine-2,3-dicarboxylic acids, 2,3,4,6,7-pentafluoro-5,8-dioxo-5,8-dihydroquinoline, and 3,4,5,6,7,8-hexafluoro-2-oxo-1,2-dihydroquinoline.
 IT 13180-38-6P
 RL: RCT (Reactant); **PREP (Preparation)**; **PREP (Preparation)**; **RACT (Reactant or reagent)** (prepn. and oxidn. of)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



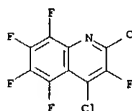
L5 ANSWER 14 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 83:131494 CA
 TITLE: Preparation of hexafluoro-1,8- and -2,7-naphthyridine
 AUTHOR(S): Van den Ham, D. M. W.
 CORPORATE SOURCE: Chem. Phys. Lab., Twente Univ. Technol., Enschede, Meth.
 SOURCE: Journal of Fluorine Chemistry (1975), 5(6), 537-44
 CODEN: JFLCAR; ISSN: 0022-1139
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB Hexachloro-1,8- (I) and -2,7-naphthyridine (II) were prepd. from 2,7-dichloro-1,8-naphthyridine and 1,3,6,8-tetrachloro-2,7-naphthyridine resp. From I and II and their starting materials a series of partially and totally fluorine substituted compds. were prepd.
 IT 56595-12-1P
 RL: SPN (Synthetic preparation); **PREP (Preparation)** (prepn. of)
 RN 56595-12-1 CA
 CN 1,8-Naphthyridine, 2,3,4,5,6,7-hexafluoro- (9CI) (CA INDEX NAME)



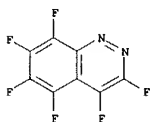
L5 ANSWER 15 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 77:19504 CA
 TITLE: Reactions involving fluoride ion. V. Synthesis of perfluoro(isopropyl)quinolines
 AUTHOR(S): Chambers, R. D.; Corbally, R. P.; Musgrave, W. K. R.; Jackson, J. A.; Matthews, R. S.
 CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1972), (9-10), 1286-90
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB F-induced reaction of F₃CCF:CF₂ with perfluoroquinoline in triglyme or tetraglyme gave a mixt. of perfluoro(isopropyl)quinolines [e.g. perfluoro(2,4-diisopropyl)quinoline] (I), substitution occurring preferentially at the 2- and 4-positions followed by attack at the 6-position. I rearranged on heating with F⁻, giving the 2,6-isomer as the main product. Unusually large coupling consts. between a 4-(CF₃)₂CF group and a 5-F atom were obsd. in the 19F NMR spectra of these compds.; the temp. dependence of the spectra was discussed in terms of preferential population of particular conformations.
 IT 36779-48-3P
 RL: SPN (Synthetic preparation); **PREP (Preparation)** (prepn. of)
 RN 36779-48-3 CA
 CN Quinoline, 3,4,5,6,7,8-hexafluoro-2-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]- (9CI) (CA INDEX NAME)



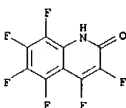
L5 ANSWER 16 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 74:53453 CA
 TITLE: Polyfluoroheterocyclic compounds. XVIII. Reactions of heptafluoroquinoline and -isoquinoline and pentafluoropyridine with hydrogen halides
 AUTHOR(S): Chambers, Richard D.; Hole, M.; Musgrave, William K. R.; Thorpe, J. G.
 CORPORATE SOURCE: Sci. Lab., Univ. Durham, Durham, UK
 SOURCE: Journal of the Chemical Society [Section] C: Organic (1971), (1), 61-7
 CODEN: JSOQAX; ISSN: 0022-4952
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB When pentafluoropyridine (I), heptafluoroquinoline (II), and heptafluoroisoquinoline (III) reacted with hydrogen halides in tetrahydrothiophene dioxide, F ortho and para to ring N was replaced by the other halogen. The order of reactivity is II >>> III > I. Reaction of II occurred at room temp. with substitution first at the 2- and then at the 4-position, to give 28-61% 2,4-dihalo derivs. Reaction of I or III required elevated temps.; I gave 4- and 2,4,6-substituted derivs., and III the 1-halo deriv. in low yields. Small amounts of H₂O in the solvent deactivated the system. The mechanism of the reactions is discussed in terms of nucleophilic displacement of fluoride ion from the protonated species.
 IT 27401-84-9P
 RL: SPN (Synthetic preparation); **PREP (Preparation)** (prepn. of)
 RN 27401-84-9 CA
 CN Quinoline, 2,4-dichloro-3,5,6,7,8-pentafluoro- (8CI, 9CI) (CA INDEX NAME)



L5 ANSWER 17 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 73:66535 CA
 TITLE: Hexafluorocinnoline: synthesis and photochemical isomerization to hexafluoroquinazoline
 AUTHOR(S): Chambers, Richard D.; MacBride, John A. H.; Musgrave, William K. R.
 CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, UK
 SOURCE: Journal of the Chemical Society [Section] D: Communications (1970), (12), 739-40
 CODEN: CCJDAO; ISSN: 0577-6171
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB Hexafluorocinnoline (I) was prepd. from hexachlorocinnoline (II) and isomerized to hexafluoroquinazoline (III) in 5-10% yields by uv irradiat.
 at
 were
 IT 29734-86-3P
 RL: RCT (Reactant); PREP (Preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and photochem. rearrangement of)
 RN 29734-86-3 CA
 CN Cinnoline, hexafluoro- (8CI, 9CI) (CA INDEX NAME)



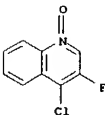
L5 ANSWER 18 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)
 refluxed 5.5 hrs. and worked up to give 0.5 g. 2-hydroxy-4-methoxy-3,5,6,7,8-pentafluoroquinoline (VIII), m. 250-63.degree. (decompn.) (CHCl3-benzene), and 0.25 g.
 2,4-dihydroxy-3,5,6,7,8-penta-fluoroquinoline (IX), m. 245-55.degree. (decompn.) (EtOAc). A mixt. of 1 g. IIIa and 1.1 g. anhyd. AlCl3 is heated 3.5 hrs. at 120.degree. and worked up to give 0.5 g. 2-hydroxy-3,4,5,6,7,8-hexafluoroquinoline (X), m. 211.degree. (decompn.) (petroleum ether-CH2Cl2); a similar demethylation of IIb with AlCl3 gives a mixt. (m. 137.5-9.5.degree. (decompn.), after sublimation
 at
 80%/0.05 mm.) contg. 80% 4-hydroxy-2,3,5,6,7,8-hexafluoroquinoline. To a soln. of 1 g. I in 20 ml. H2SO4 (sp. gr. 1.84) is added dropwise 100 ml. H2O over 0.5 hr., and the ppt. (0.8 g.) filtered off and sublimed at 110.degree./0.1 mm. to give X. Excess CH2N2 in dry Et2O is added to a suspension of 2.35 g. IX in 300 ml. dry Et2O, and the mixt. worked up to give 2.1 g. of a 9:10 mixt., sep'd. by fractional sublimation and recrystn., of IV and 4-methoxy-1-methyl-3,5,6,7,8-pentafluoro-2(1H)-quinolone (XI), m. 115-16.degree.; IV and XI are also obtained in a 4:5 ratio by similarly methylating VIII, while X gives IIIa and 1-methyl-3,4,5,6,7,8-hexafluoro-2(1H)-quinolone (XII), m. 127-7.4.degree., in 2:3 ratio. A stirred mixt. of 2 g. I and 0.88 g. KOH in 50 ml. H2O is refluxed 4.25 hrs., and worked up via CH2N2 to give 1.4 g. of a mixt. of 30% IIIa, 20% IIIb and 50% XII; an analogous reaction in Me3COH gives a mixt. of 32% IIIa, 6% IIIb, and 62% XII with the same amt. of KOH, and a mixt. of 40% IIIa, 2% IIIb, 38% XII, 15% IV, and 5% XI with half again
 the
 amt. KOH. MeOH (150 ml.) is added dropwise over 1 hr. to a soln. of 1 g. I in 20 ml. H2SO4 (sp. gr. 1.84) at 0.degree., the soln. shaken with CH2Cl2, 150 ml. H2O added slowly over 1 hr., and the mixt. worked up to give 0.55 g. of a 3:17 mixt. of I and IIIa, and 0.1 g. X.
 IT 13180-42-2P
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
 RN 13180-42-2 CA
 CN 2(1H)-Quinolone, 3,4,5,6,7,8-hexafluoro- (9CI) (CA INDEX NAME)



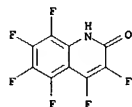
L5 ANSWER 18 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 71:81210 CA
 TITLE: Heptafluoroquinoline and derivatives
 INVENTOR(S): Chambers, Richard D.; Hole, Michael; Musgrave, William
 K. R.
 PATENT ASSIGNEE(S): National Research Development Corp.
 SOURCE: Brit., 7 pp.
 CODEN: BRXXAA
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1155965		19690625	GB	19650513

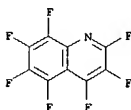
GI For diagram(s), see printed CA Issue.
 AB The title compds. are prepd. Thus, an intimate mixt. of 31 g. heptachloroquinoline [m. 155-7.degree. (benzene), prepd. in 78% yield from 95.5 g. tetra-chloroquinoline and 1054 g. PC15 at 315-30.degree.] and 72.5 g. anhyd. KF is heated 17 hrs. at 470.degree. in vacuo to give 18 g. of a mixt. of 85% heptafluoroquinoline (I), b. 205-5.5.degree., m. 95-5.5.degree.; 12% chlorohexafluoroquinoline isomer (II), m. 89-90.degree.; and 3% isomer of II. A soln. of 0.1 g. Na in dry MeOH is added slowly to a stirred mixt. of 1.14 g. I in 12 ml. dry MeOH, and the mixt. stirred 15 min. and worked up to give 0.91 g. of a mixt. of 97% methoxyhexafluoroquinolines [3.4:1 mixt. of IIIa-IIIb (defined below)],
 2% I, and 1% 2,4-dimethoxy-3,5,6,7,8-pentafluoro-quinoline (IV), m. 107.5-8.5.degree. (MeOH), sep'd. to give 2-methoxy-3,4,5,6,7,8-hexafluoroquinoline (IIIa), m. 50.5-1.5.degree., and 4-methoxy-2,3,5,6,7,8-hexafluoroquinoline (IIIb), m. 68.5-69.degree.; similar expts. with other proportions of Na give IIIa, IV, and (probably) a >9:1 mixt. of 2,4,7- and 2,4,6-trimethoxytetra-fluoroquinolines, glassy at 123-35.degree., m. 135-6.degree.. A soln. of 1.28 g. N2H4.H2O in 5 ml. dioxane is added over 35 min. to a stirred soln. of 30.9 g. I in 20 ml. dioxane at 20.degree., and the mixt. stirred 45 min. and worked up to give 2.95 g. solid, sublimed in vacuo to give 76% 2-hydrazino-3,4,5,6,7,8-hexafluoroquinoline (VI), decompd. 196.degree.. A soln. of 3.85 g. CuSO4.5H2O (VI) in 70 ml. H2O is added slowly over 45 min. to a suspension of 2.22 g. V in 50 ml. H2O, a soln. of 1.2 g. VI in 10 ml. H2O added, and the mixt. refluxed 1 hr. and worked up to give 0.5 g. solid, sublimed at 20-30.degree./0.1 mm. to give 3,4,5,6,7,8-hexafluoroquinoline, m. 62.5-4.5.degree.. Aq. NH3 (sp. gr. 0.88) (1 ml.) is added to a stirred soln. of 1 g. I in 10 ml. Me2CO at 20.degree., and the mixt. stirred 45 min. and worked up to give 0.9 g. solid, recrystd. (Me2CO-CH2Cl2) and sublimed in vacuo to give 2-amino-3,4,5,6,7,8-hexafluoroquinoline (VII), m. 224-5.degree., and a 1:4 mixt., m. 158.5-60.degree., of VII and 4-amino-2,3,5,6,7,8-hexafluoroquinoline. A mixt. of 1.25 g. IV and 15 ml. 54% aq. HI is



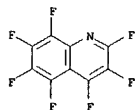
L5 ANSWER 20 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 66:46302 CA
 TITLE: Polyfluoroheterocyclic compounds. IX. Tautomerism
 in
 polyfluorohydroxyquinolines and -isoquinolines
 AUTHOR(S): Chambers, Richard D.; Hole, Michael; Musgrave,
 William
 CORPORATE SOURCE: K. R.; Storey, R. A.
 Univ. Sci. Labs., Durham, UK
 SOURCE: Journal of the Chemical Society [Section] C: Organic
 (1967), (1), 53-7
 CODEN: JSOQAX; ISSN: 0022-4952
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB cf. CA 66, 28627w. Heptafluoroquinoline with aq. NaOH or with KOH in
 tert-BuOH gives a mixt. of 2-and 4-hydroxyhexafluoroquinolines;
 heptafluoroisoquinoline reacts to give the 1-hydroxy deriv.
 2-Hydroxyhexafluoroquinoline (I) and 1-hydroxyhexafluoroisoquinoline
 exist
 as tautomers and react with CH₂N₂ giving a mixt. of O- and N-Me derivs.
 whereas 4-hydroxyhexafluoroquinoline gives only an O-Me deriv. The
 factors affecting tautomerism in these systems are outlined.
 IT 13180-42-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 13180-42-2 CA
 CN 2(1H)-Quinolinone, 3,4,5,6,7,8-hexafluoro- (9CI) (CA INDEX NAME)



L5 ANSWER 21 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 66:28627 CA
 TITLE: Polyfluoro heterocyclic compounds. VIII.
 Nucleophilic substitution in heptafluoroquinoline and
 -isoquinoline
 AUTHOR(S): Chambers, Richard D.; Hole, Michael; Musgrave,
 William
 CORPORATE SOURCE: K. R.; Storey, R. A.; Iddon, Brian
 Univ. Sci. Labs., Durham, UK
 SOURCE: Journal of the Chemical Society [Section] C: Organic
 (1966), (24), 2331-9
 CODEN: JSOQAX; ISSN: 0022-4952
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB cf. preceding abstr. Nucleophilic substitution in heptafluoroquinoline
 and (or) heptafluoroisoquinoline by various nucleophiles, e.g., sodium
 methoxide, ammonia, hydrazine, and LiAlH₄ is described. Monosubstitution
 and disubstitution in heptafluoroquinoline occurs at the 2-and
 4-positions
 while in heptafluoroisoquinoline attack occurs first, specifically, at
 the
 1-position and then at the 6-position. Oxidn. of heptafluoroisoquinoline
 and the methoxy derivs. gives tri- and difluoropyridinedicarboxylic acids
 which aid the analysis of the 19F N.M.R. spectra of the methoxy derivs.
 and establish their structures. Analysis of the 19F N.M.R. spectra of
 the
 derivs. of heptafluoroquinoline also clearly distinguishes their
 structures. In both series, some very large coupling consts. are
 observed
 which are assigned to peri F-F coupling. The major factor detg. the
 orientation of nucleophilic substitution in these systems is the effect
 of
 the ring nitrogen on the relative stabilities of the transition states.
 IT 13180-38-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



L5 ANSWER 22 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 66:28626 CA
 TITLE: Polyfluoro heterocyclic compounds. VII.
 Heptafluoroquinoline and -isoquinoline
 AUTHOR(S): Chambers, Richard D.; Hole, Michael; Iddon, Brian;
 Musgrave, William K. R.; Storey, R. A.
 CORPORATE SOURCE: Univ. Sci. Labs., Durham, UK
 SOURCE: Journal of the Chemical Society [Section] C: Organic
 (1966), (24), 2328-31
 CODEN: JSOQAX; ISSN: 0022-4952
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB cf. CA 64, 7986c. Heptachloroquinoline and -iso-quinoline have been
 prepd. by initial direct chlorination of quinoline and isoquinoline and
 subsequent reaction of the products with PO₅ at elevated temps. Reaction
 of these perchloro compds. with KF at elevated temps. gives
 heptafluoroquinoline (I) and -isoquinoline in good yields. The perhalo
 quinolines and isoquinolines show no basic properties except that they
 dissolve in concd. sulfuric acid, and that the soln. of
 heptafluoroquinoline on slow addn. of water or methanol gives the
 monohydroxy or -methoxy derivs. but on rapid diln. gives
 heptafluoroquinoline. The mechanism of the reaction is discussed in
 terms
 of nucleophilic displacement of fluoride ion from the protonated species.
 IT 13180-38-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



10/607,220

=> s l4 not l5

L6 18 L4 NOT L5

=> d ibib abs fhitstr hitrn 1-18

10/607,220

L6 ANSWER 1 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 140:235614 CA
 TITLE: Quinolyl propyl piperidine derivatives, the preparation thereof and compositions containing same, useful as antimicrobials
 INVENTOR(S): Bacque, Eric; Bigot, Antony; El Ahmad, Youssef; Malleron, Jean Luc; Mignani, Serge; Ronan, Baptiste; Tabart, Michel; Viviani, Fabrice
 PATENT ASSIGNEE(S): Aventis Pharma SA, Fr.
 SOURCE: Fr. Demande, 66 pp.
 CODEN: FRXXBL
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2844270	A1	20040312	FR 2002-11212	20020911
WO 2004024712	A1	20040325	WO 2003-FR2686	20030910
W: AE, AG, AL, AU, BA, BB, BR, BZ, CA, CN, CO, CR, CU, DM, DZ, EC, GE, GR, HR, HU, ID, IL, IN, IS, JP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NI, NO, NZ, OM, PG, PH, PL, RO, SC, SG, SI, TN, TT, UA, UZ, VC, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004067619	A1	20040506	US 2003-659164	20030910
PRIORITY APPL. INFO.:			FR 2002-11212	A 20020911
OTHER SOURCE(S):	MARPAT 140:235614			
GI				

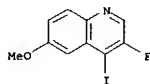
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB New 4-[3-(Quinol-4-yl)propyl]piperidine derivs. I are disclosed [wherein R1 = H or F; R2 = COOH, CH2CO2H, CH2OH; R3 = Cl-6 alkyl substituted by: (un)substituted Sph [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by 3- to 7-membered cycloalkylthio, or by 5- to 6-membered arom. heterocyclylthio comprising 1-4 N/O/S atoms and optionally substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2; or R3 = propargyl substituted by: Ph [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by cycloalkyl contg. 3-7 members, or by 5- to 6-membered arom. heterocyclyl with 1-4 N/O/S atoms [and (un)substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2]; R4 = Cl-6 alkyl, alkenyl-CH2, or alkynyl-CH2 (alkenyls or alkynyls comprise 2-6 C atoms), cycloalkyl, or cycloalkylalkyl (cycloalkyls comprises 3-8 C atoms); including

L6 ANSWER 2 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 137:232568 CA
 TITLE: Quinolyl propyl piperidine derivatives, the preparation thereof and compositions containing same, useful as antimicrobials
 INVENTOR(S): Bacque, Eric; Mignani, Serge; Malleron, Jean-Luc; Tabart, Michel; Evers, Michel; Viviani, Fabrice; El-Ahmad, Youssef; Mutti, Stephane; Daubie, Christophe
 PATENT ASSIGNEE(S): Aventis Pharma S.A., Fr.
 SOURCE: PCT Int. Appl., 71 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

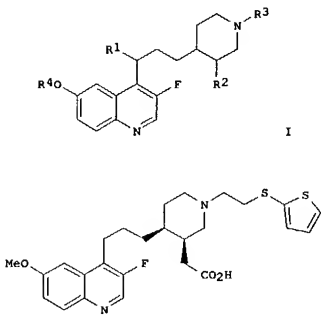
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002072572	A1	20020919	WO 2002-FR851	20020311
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GR, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AE, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
FR 2822154	A1	20020920	FR 2001-3374	20010313
EP 1370550	A1	20031217	EP 2002-722329	20020311
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, NL, SE, MC, PT, IS, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2002177606	A1	20021128	US 2002-96482	20020313
US 6602884	B2	20030805		
US 2003171369	A1	20030911	US 2003-387479	20030314
PRIORITY APPL. INFO.:			FR 2001-3374	A 20010313
			US 2001-281407P	P 20010405
			WO 2002-FR851	W 20020311
			US 2002-96482	A3 20020313
OTHER SOURCE(S):	MARPAT 137:232568			
GI				

L6 ANSWER 1 OF 18 CA COPYRIGHT 2004 ACS on STN (Continued)
 enantiomeric and diastereoisomeric forms, mixts. thereof, and salts thereof]. The novel derivs. are particularly interesting as antimicrobial agents. Five synthetic examples are given. For example, II was prepd. by N-alkylation of III (prepn. given) with 2-[(2-bromoethyl)sulfanyl]-1,4-difluorobenzene, followed by acidic hydrolysis. Comps. I were active against exptl. infections of mice by Staphylococcus aureus IP 8203 at 12-150 mg/kg s.c., and at 26-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c. (2 administrations).
 IT 426842-84-4, 4-Iodo-3-fluoro-6-methoxyquinoline
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of quinolylpropylpiperidines as antimicrobials)
 RN 426842-84-4 CA
 CN Quinoline, 3-fluoro-4-iodo-6-methoxy- (9CI) (CA INDEX NAME)



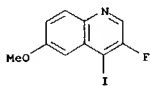
IT 426842-84-4, 4-Iodo-3-fluoro-6-methoxyquinoline
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of quinolylpropylpiperidines as antimicrobials)
 REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L6 ANSWER 2 OF 18 CA COPYRIGHT 2004 ACS on STN (Continued)



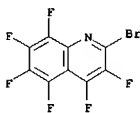
AB New 4-[3-(Quinol-4-yl)propyl]piperidine derivs. I are disclosed [wherein R1 = H, halo, OH, NH2, alkylamino, dialkylamino, hydroxyamino, alkoxyamino, or alkylalkoxyamino; R2 = COOH, CH2CO2H, CH2OH; R3 = Cl-6 alkyl substituted by: (un)substituted Sph [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by 3- to 7-membered cycloalkylthio, or by 5- to 6-membered arom. heterocyclylthio comprising 1-4 N/O/S atoms and optionally substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2; or R3 = propargyl substituted by: Ph [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by cycloalkyl contg. 3-7 members, or by 5- to 6-membered arom. heterocyclyl with 1-4 N/O/S atoms [and (un)substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2]; R4 = Cl-6 alkyl, alkenyl-CH2, or alkynyl-CH2 (alkenyls or alkynyls comprise 2-6 C atoms), cycloalkyl, or cycloalkylalkyl (cycloalkyls comprises 3-8 C atoms); including diastereoisomeric forms, mixts. thereof, cis or trans forms, and salts thereof]. The novel derivs. are particularly interesting as antimicrobial agents. Ten synthetic examples are given. For instance, Wittig reaction of 4(RS)-4-allyl-1-(benzyloxycarbonyl)piperidin-3-one with Ph3P:CHCO2Me gave a Z-isomeric exocyclic olefin, which underwent hydroboration at allyl and Pd-catalyzed coupling with 4-iodo-3-fluoro-6-methoxyquinoline, followed by hydrogenation of the olefin with concomitant N-deprotection, N-alkylation with 2-[(2-bromoethylthio)thiophene, and sapon. of the Me ester, to give the racemic title compd. II.2HCl. Comps. I were active against exptl. infections of mice by Staphylococcus aureus IP 8203 at 12-150 mg/kg s.c., and at 26-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c. (2 administrations).
 IT 426842-84-4, 4-Iodo-3-fluoro-6-methoxyquinoline

L6 ANSWER 2 OF 18 CA COPYRIGHT 2004 ACS on STN (Continued)
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (precursor; prepn. of (quinolylpropyl)piperidine derivs. as
 antimicrobials)
 RN 426842-84-4 CA
 CN Quinoline, 3-fluoro-4-iodo-6-methoxy- (9CI) (CA INDEX NAME)



IT 426842-84-4, 4-Iodo-3-fluoro-6-methoxyquinoline
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (precursor; prepn. of (quinolylpropyl)piperidine derivs. as
 antimicrobials)
 REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L6 ANSWER 3 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 137:62929 CA
 TITLE: DFT Calculation of NMR JFF Spin-Spin Coupling
 Constants in Fluorinated Pyridines
 AUTHOR(S): Barone, Veronica; Peralta, Juan E.; Contreras, Ruben
 H.; Snyder, James P.
 CORPORATE SOURCE: Departamento de Fisica FCEYN, Universidad de Buenos
 Aires, Buenos Aires, Argent.
 SOURCE: Journal of Physical Chemistry A (2002), 106(23),
 5607-5612
 CODEN: JPCAFH; ISSN: 1089-5639
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB All four isotropic contributions to the NMR fluorine-fluorine coupling
 consts. (Fermi contact, FC, spin-dipolar, SD, paramagnetic spin-orbit,
 PSO, and diamagnetic spin-orbit, DSO) have been calcd. for
 2,6-difluoropyridine, 2,4,6-trifluoropyridine, perfluoropyridine, and
 2-Br-3,4,5,6,7,8-hexafluoroquinoline by means of d. functional theory in
 combination with the rather modest 6-311G** basis set. Exptl. values
 ranging from -20.3 to +45.8 Hz are semiquant. reproduced for three- to
 seven-bond couplings, suggesting that the different electronic effects
 responsible for the spin-spin interactions are adequately taken into
 account. In all cases, the relative importance of noncontact terms was
 examd. With few exceptions, the sum of the SD and PSO noncontact terms
 is
 larger than the FC contact contribution, even though in most cases the
 two
 noncontact values have opposite signs. The widespread assumption that
 the
 Fermi contact term dominates scalar spin-spin couplings in the case of
 light atoms would appear to be an oversimplification for JFF in
 polyfluorinated org. mols. In addn., the CPU performance of the Fermi
 contact contribution calcd. sep. by the coupled-perturbed and the
 finite-perturbation methods was investigated showing the latter to be
 slightly more efficient.
 IT 60870-78-2, 2-Bromohexafluoroquinoline
 RL: PEP (Physical, engineering or chemical process); PRP (Properties);
 PYP (Physical process); PROC (Process)
 (DFT calcn. of NMR spin-spin coupling consts. in fluorinated
 pyridines)
 RN 60870-78-2 CA
 CN Quinoline, 2-bromo-3,4,5,6,7,8-hexafluoro- (9CI) (CA INDEX NAME)



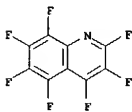
IT 60870-78-2, 2-Bromohexafluoroquinoline

L6 ANSWER 3 OF 18 CA COPYRIGHT 2004 ACS on STN (Continued)
 RL: PEP (Physical, engineering or chemical process); PRP (Properties);
 PYP (Physical process); PROC (Process)
 (DFT calcn. of NMR spin-spin coupling consts. in fluorinated
 pyridines)
 REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L6 ANSWER 4 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 119:206380 CA
 TITLE: Extraction of perfluoroalkyl sulfonyl fluoride
 INVENTOR(S): Sato, Yukio
 PATENT ASSIGNEE(S): Tookemu Purodakutsu Kk, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKKXAF
 Patent
 Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05168844	A2	19930702	JP 1991-65523	19910306
JP 3030661	B2	20000410		

PRIORITY APPL. INFO.: JP 1991-65523 19910306
 AB Perfluoroalkyl sulfonyl fluoride CnF2n+1SO2F (n=2-5) in F-contg. inert
 solvents is extd. by contacting with an aq. or alc. soln. contg. inert
 hydroxide
 or carbonate of alkali or alk. earth metals, preferably selected from
 KOH,
 NaOH, LiOH, Ba(OH)2, K2CO3, or Li2CO3.
 IT 13180-38-6, Perfluoroquinoline
 RL: USES (Uses)
 (extn. of perfluoroalkyl sulfonic fluoride from, by potassium
 hydroxide
 soln.)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



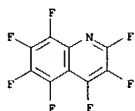
IT 13180-38-6, Perfluoroquinoline
 RL: USES (Uses)
 (extn. of perfluoroalkyl sulfonic fluoride from, by potassium
 hydroxide
 soln.)

10/607,220

L6 ANSWER 5 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 119:206379 CA
 TITLE: Separation of perfluoroalkyl sulfonyl fluoride
 INVENTOR(S): Sato, Yukio
 PATENT ASSIGNEE(S): Tookemu Purodakutsu Kk, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

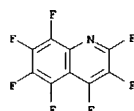
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05168843	A2	19930702	JP 1991-65517	19910306
JP 3030660	B2	20000410		

PRIORITY APPLN. INFO.: JP 1991-65517 19910306
 AB A gas contg. perfluoroalkyl sulfonic fluoride (I) $C_nF_{2n+1}SO_2F$ ($n=2-5$) is contacted with a F-contg. inert solvent as an absorbent to sep. I. The gas contg. I is produced by electrolytic fluorination of alkyl sulfonic acid, alkylsulfonic fluoride, or alkylsulfonic chloride.
 IT 13180-38-6, Perfluoroquinoline
 RL: USES (Uses)
 (absorbent, sepn. of perfluoroalkyl sulfonic fluoride by, from reaction gas mixts.)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



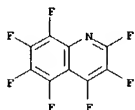
IT 13180-38-6, Perfluoroquinoline
 RL: USES (Uses)
 (absorbent, sepn. of perfluoroalkyl sulfonic fluoride by, from reaction gas mixts.)

L6 ANSWER 6 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 95:167967 CA
 TITLE: Proton-proton inter-ring coupling constants in isoquinoline and quinazoline. Their relationship with corresponding fluorine-19-fluorine-19 couplings in perfluoro derivatives
 AUTHOR(S): Cassidei, L.; Sciacovelli, O.
 CORPORATE SOURCE: Ist. Chim. Fis., Univ. Bari, Bari, 70126, Italy
 SOURCE: Journal of Magnetic Resonance (1969-1992) (1981), 44(2), 340-7
 CODEN: JOMRA4; ISSN: 0022-2364
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Complete spectral anal. of ^{1}H NMR of isoquinoline and quinazoline is performed. Signs of interfering coupling constns. (JHHir) are detd. by INDOR expts. The mechanisms of transmission of JHHir are discussed. A linear correlation exists between the majority of JHHir of quinoline, isoquinoline, and quinazoline and JFFir of their perfluoro derivs.; exceptions are rationalized. The linear relationship, with the near-zero value of intercept, strongly suggests that JFFir originate, almost quant. from the Fermi contact term and are transmitted via the .pi.-electron system, except for the peri JFFir. A calcn. of the proportionality between JHHir and JFFir in quinoline, using the Pople and Santry expression for the contribution of .pi. electrons to interring coupling constns., agrees with the exptl. data.
 IT 13180-38-6
 RL: PRP (Properties)
 (interring proton coupling const. in quinoline vs.)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



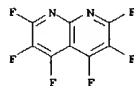
IT 13180-38-6
 RL: PRP (Properties)
 (interring proton coupling const. in quinoline vs.)

L6 ANSWER 7 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 91:90752 CA
 TITLE: Relationship between proton-proton and fluorine-19-fluorine-19 inter-ring coupling constants in fused aza aromatic systems
 AUTHOR(S): Cassidei, L.; Dell'Atti, A.; Sciacovelli, O.
 CORPORATE SOURCE: Ist. Chim. Fis., Univ. Bari, Bari, 70100, Italy
 SOURCE: Spectroscopy Letters (1979), 12(5), 365-9
 CODEN: SPLEBX; ISSN: 0038-7010
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Inter-ring coupling constns. (JFF and JHH) in quinoline, isoquinoline, and the corresponding perfluoro derivs. were detd. The data indicate that JFF are transmitted only through .pi.-electrons and large stereospecific .sigma.-contributions transmitted through the all-trans pathway are absent in F-F coupling.
 IT 13180-38-6
 RL: PRP (Properties)
 (fluorine-fluorine coupling constns. in)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



IT 13180-38-6
 RL: PRP (Properties)
 (fluorine-fluorine coupling constns. in)

L6 ANSWER 8 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 91:67917 CA
 TITLE: Rapid general microdetermination of fluorine
 AUTHOR(S): Van Leuven, H. C. E.; Rotscheid, G. J.; Buis, W. J.
 CORPORATE SOURCE: K./Shell Lab., Amsterdam, Neth.
 SOURCE: Fresenius' Zeitschrift fuer Analytische Chemie (1979), 296(1), 36-9
 CODEN: ZACFAU; ISSN: 0016-1152
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A rapid micromethod for the detn. of F in a wide variety of materials is based on the liberation of F as HF from the sample by means of pyrohydrolysis with steam at 1120.degree.. The amt. of F in the condensate is subsequently measured with an ion-selective electrode by using a simple std. addn. technique, which automatically compensates for variations in ionic strength, acidity, etc. Metals that may form stable complexes with fluoride are masked by the addn. of a complexing agent to the condensate. Materials analyzed included org. and organometallic compds., alumina-base catalysts, coal, etc. The limit of detection is of the order of 1 .mu.g F; the std. deviation is about 1% relative. The time required for one detn. is 15-20 min.
 IT 56595-12-1
 RL: AMX (Analytical matrix); ANST (Analytical study)
 (fluorine detn. in, by pyrohydrolysis and subsequent potentiometry)
 RN 56595-12-1 CA
 CN 1,8-Naphthyridine, 2,3,4,5,6,7-hexafluoro- (9CI) (CA INDEX NAME)



IT 56595-12-1
 RL: AMX (Analytical matrix); ANST (Analytical study)
 (fluorine detn. in, by pyrohydrolysis and subsequent potentiometry)

L6 ANSWER 9 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 87:4858 CA
 TITLE: Fluorine-19 NMR spectra of heptafluoroisoquinoline
 and

hexafluoro-1-methoxyisoquinoline. Long-range
 inter-ring coupling constants
 AUTHOR(S): Matthews, R. S.
 CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, UK
 SOURCE: Organic Magnetic Resonance (1976), 8(12), 628-31
 CODEN: ORMRBD; ISSN: 0030-4921

DOCUMENT TYPE: Journal
 LANGUAGE: English

AB An anal. of the 19F NMR spectra of heptafluoroisoquinoline and
 hexafluoro-1-methoxyisoquinoline is presented. The inter-ring F-F
 coupling constns. alternate in sign and magnitude and are pos. over an odd
 no. of bonds. They correlated with SCFMO C-C polarizabilities inferring
 that the long-range coupling mechanism is dominated by the contribution
 from the .pi.-electron system.

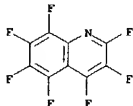
IT 13180-38-6

RL: PRP (Properties)

(bond polarizability and .pi.-bond order of, MO calcn. of)

RN 13180-38-6 CA

CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



IT 13180-38-6

RL: PRP (Properties)

(bond polarizability and .pi.-bond order of, MO calcn. of)

L6 ANSWER 10 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 85:176425 CA
 TITLE: Fluorine-19 NMR spectra of polyfluoroquinolines.
 Long

range interring fluorine-19-fluorine-19 coupling
 constants and fluorine-19 chemical shifts
 AUTHOR(S): Matthews, R. S.
 CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, UK
 SOURCE: Organic Magnetic Resonance (1976), 8(5), 240-5
 CODEN: ORMRBD; ISSN: 0030-4921

DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The signs and magnitudes of F-F coupling constns. in perfluoroquinoline
 (1), 2,4-dichloropentafluoroquinoline, and 2-bromohexafluoroquinoline were
 detd. by 19F NMR, providing unambiguous assignment of the spectra of I

and

derivs. Inter-ring F-F coupling constns. were pos. over an odd no. of
 bonds, and neg. over an even no. The 19F chem. shifts of I and I.F3CCO2H
 are reported and directly correlated with SCF MO calcd. .pi.-electron ds.
 at F and bonded C atoms.

IT 60870-79-3

RL: PROC (Process)

(fluorine-19 NMR of)

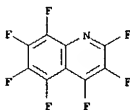
RN 60870-79-3 CA

CN Quinoline, heptafluoro-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 13180-38-6

CMF C9 F7 N



CM 2

CRN 76-05-1

CMF C2 H F3 O2



IT 60870-79-3

RL: PROC (Process)

L6 ANSWER 10 OF 18 CA COPYRIGHT 2004 ACS on STN (Continued)
 (fluorine-19 NMR of)

IT 13180-38-6 27401-84-9 60870-78-2

RL: PRP (Properties)

(fluorine-fluorine spin coupling constns. in)

L6 ANSWER 11 OF 18 CA COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 84:4155 CA

TITLE: Electrochemical reduction of azaaromatics. V.
 Influence of fluorine substitution on the electron
 affinities

AUTHOR(S): Van den Ham, D. M. W.; Harrison, G. F. S.; Spaans,
 A.;

CORPORATE SOURCE: Van der Meer, D.
 Chem. Phys. Lab., Twente Univ. Technol., Enschede,
 Neth.

SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1975),
 94(7), 168-73

CODEN: RTCPA3; ISSN: 0165-0513

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The electrochem. redn. process of fluoro-substituted azaaromatics, e.g.,
 3,6-difluoropyridazine, is described by the pattern which is normally
 postulated for aryl halogenides, that is, fission of the C-halogen bond.
 However, the stability of the intermediate mononegative ions is generally
 higher than for the comparable fluoro-substituted arenes. As an example
 of this stability, the ERS spectrum of tetrafluoroquinoxaline is given.
 The half-wave redn. potentials of the first redn. wave are related to the
 electron affinities of the molecules. These electron affinities are
 correlated with those obtained by semi-empirical quantum chem. calcs.

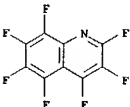
IT 13180-38-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(electrochem. redn. of, electron affinity in relation to)

RN 13180-38-6 CA

CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)

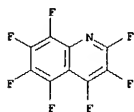


IT 13180-38-6

RL: RCT (Reactant); RACT (Reactant or reagent)

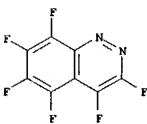
(electrochem. redn. of, electron affinity in relation to)

L6 ANSWER 12 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 83:114335 CA
 TITLE: Reactions involving fluoride ion. XII. Reactions of polyfluoro aromatic compounds with octafluorobut-2-ene
 AUTHOR(S): Chambers, R. D.; Jackson, J. A.; Partington, S.; Philpot, P. D.; Young, A. C.
 CORPORATE SOURCE: Dep. Chem., Univ. Sci. Lab., Durham, UK
 SOURCE: Journal of Fluorine Chemistry (1975), 6(1), 5-18
 CODEN: JFLCAR; ISSN: 0022-1139
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Octafluorobut-2-ene is much more difficult to dimerize, with fluoride ion, than is hexafluoropropene but perfluoro-3,4-dimethylhex-3-ene is obtained under more forcing conditions. Polyfluoroalkylations with octafluorobut-2-ene are very efficient and results with perfluoropyridine, -pyridazine, and -pyrimidine, and quinoline are described, giving various perfluoro-2-butyl derivs. Reactions with nitropentafluorobenzene and perfluorotoluene are also described. The ¹⁹F NMR spectra of perfluoro-2-butylaromatic compds. reveal restricted rotation, even at room temp.
 IT 13180-38-6
 RL: RCT (Reactant); RACT (Reactant or reagent) (perfluoroalkylation of, with octafluorobutene in presence of fluoride ion)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



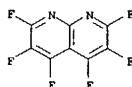
IT 13180-38-6
 RL: RCT (Reactant); RACT (Reactant or reagent) (perfluoroalkylation of, with octafluorobutene in presence of fluoride ion)

L6 ANSWER 14 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 80:2917 CA
 TITLE: Photoelectron spectra of some fluorine substituted diazanaphthalenes
 AUTHOR(S): Van den Ham, D. M. W.; Van der Meer, D.
 CORPORATE SOURCE: Chem. Phys. Lab., Twente Univ. Technol., Enschede, Neth.
 SOURCE: Journal of Electron Spectroscopy and Related Phenomena (1973), 2(3), 247-58
 CODEN: JESRAW; ISSN: 0368-2048
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The high resolution He 584 .ANG. photoelectron spectra of unsubstituted and fluorine-substituted 1,2-, 1,3-, 1,4- and 2,3-diazanaphthalenes are presented. F substitution enables more definite anal. of the photoelectron spectra of the parent compds. Unexpected shifts of the N lone-pair bands can be explained within the through-space and through-bond interaction model and it was deduced that F substitution can give expl. evidence about the sym. character of the lone-pair MO.
 IT 28734-86-3
 RL: PRP (Properties) (photoelectron spectrum of)
 RN 28734-86-3 CA
 CN Cinnoline, hexafluoro- (8CI, 9CI) (CA INDEX NAME)



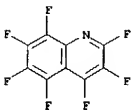
IT 28734-86-3
 RL: PRP (Properties) (photoelectron spectrum of)

L6 ANSWER 13 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 83:105955 CA
 TITLE: Photoelectron spectra of fluorine substituted diazanaphthalenes. Even cases
 AUTHOR(S): Van den Ham, D. M. W.; Beerlage, M.; Van der Meer, D.; Fell, D.
 CORPORATE SOURCE: Chem. Phys. Lab., Twente Univ. Technol., Enschede, Neth.
 SOURCE: Journal of Electron Spectroscopy and Related Phenomena (1975), 7(1), 33-43
 CODEN: JESRAW; ISSN: 0368-2048
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The high resolution He 584 .ANG. photoelectron spectra of 3 diazanaphthalenes and some of their fluoro deriva. are presented. The qualitative model that is used frequently in the discussion of lone-pair level splittings was examd.
 IT 56595-12-1
 RL: PRP (Properties) (uv photoelectron spectrum and ionization potential of)
 RN 56595-12-1 CA
 CN 1,8-Naphthyridine, 2,3,4,5,6,7-hexafluoro- (9CI) (CA INDEX NAME)



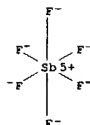
IT 56595-12-1
 RL: PRP (Properties) (uv photoelectron spectrum and ionization potential of)

L6 ANSWER 15 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 77:132989 CA
 TITLE: Perfluoro effect in the photoelectron spectra of quinoline and isoquinoline
 AUTHOR(S): Van den Ham, D. M. W.; Van der Meer, D.
 CORPORATE SOURCE: Chem. Phys. Lab., Twente Univ. Technol., Enschede, Neth.
 SOURCE: Chemical Physics Letters (1972), 15(4), 549-52
 CODEN: CHPLBC; ISSN: 0009-2614
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The high-resoln. He 584 .ANG. photoelectron spectra of heptafluoroquinoline and heptafluoroisoquinoline are compared with those of the parent compds. Shifts in pi-ionization potentials, due to the F substitution, can be described with an inductive and a combined inductive-conjugative Hueckel model.
 IT 13180-38-6
 RL: PRP (Properties) (photoelectron spectrum of, fluorine substitution effects in relation to)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



IT 13180-38-6
 RL: PRP (Properties) (photoelectron spectrum of, fluorine substitution effects in relation to)

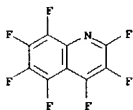
L6 ANSWER 16 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 75:117851 CA
 TITLE: Polyfluoro-heterocyclic compounds. XIX. Relative base strengths of some polyfluoroaryl-nitrogen heterocyclic systems
 AUTHOR(S): Bell, S. L.; Chambers, R. D.; Musgrave, W. K. R.; Thorpe, J. G.
 CORPORATE SOURCE: Dep. Chem., Univ. Sci. Lab., Durham, UK
 SOURCE: Journal of Fluorine Chemistry (1971), 1(1), 51-7
 CODEN: JFLCAR; ISSN: 0022-1139
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A series of hexafluoroantimonate salts of perfluoropyridine, perfluoroquinoline, perfluoroisoquinoline, and perfluoropyrazine, and of 3,5-dichlorofluoropyridine were isolated. A relative order of base strength was obtained from ^{19}F NMR measurements on mixts. of bases with acid which indicated that a dominant factor affecting base strength was the no. of F atoms ortho to the N atom.
 IT 33808-40-1
 RL: PRP (Properties)
 (basicity of, N.M.R. in relation to)
 RN 33808-40-1 CA
 CN Antimonate(1-), hexafluoro-, (OC-6-11)-, hydrogen, compd. with heptafluoroquinoline (1:1) (9CI) (CA INDEX NAME)
 CM 1
 CRN 16930-06-4
 CMP F6 Sb . H
 CCI CCS



● H⁺

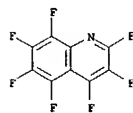
CM 2
 CRN 13180-38-6
 CMP C9 F7 N

L6 ANSWER 17 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 71:61301 CA
 TITLE: Acid catalyzed nucleophilic substitutions in heterocyclic systems
 AUTHOR(S): Musgrave, William K. R.
 CORPORATE SOURCE: Univ. Durham, Durham, UK
 SOURCE: Chemistry & Industry (London, United Kingdom) (1969), (28), 943-7
 CODEN: CHINAG; ISSN: 0009-3068
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB Perfluoroquinoline (I) reacted with anhyd. HCl in dried sulfolane to give 2-chlorohexafluoroquinoline, 2,4-dichloro-pentafluoroquinoline, and 2-chloro-4-hydroxypentafluoroquinoline. The latter was absent when sulfolane dried over mol. sieves was used. HBr gave the corresponding products only when rigorously dry sulfolane was used. Very little substitution was shown by pentafluoropyridine treated with HCl and HBr as above; however, tetrafluoropyridazine (II) was more susceptible to nucleophilic substitution, the F in positions 4 and 5 reacting 1st, while in acid soln. 3-F and 6-F were replaced 1st. When HCl was bubbled through II in Et₂O, all 4-F atoms were replaced. AlCl₃ and AlBr₃ reacted with I at 150.degree. to give only 2-substituted products, but AlBr₃ at >150.degree. and AlI₃ at 150.degree. gave 2,8-disubstituted derivs. Pentafluoropyridine decompd. when heated with Al halides; however, when the corresponding halogen acid was added, the same products were obtained as in the reactions involving the halogen acid alone.
 IT 13180-38-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (substitution reaction of, mechanism of)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



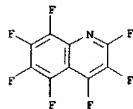
IT 13180-38-6 27401-84-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (substitution reaction of, mechanism of)

L6 ANSWER 16 OF 18 CA COPYRIGHT 2004 ACS on STN (Continued)



IT 33808-40-1
 RL: PRP (Properties)
 (basicity of, N.M.R. in relation to)
 IT 13180-38-6
 RL: PRP (Properties)
 (nuclear magnetic resonance of)

L6 ANSWER 18 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 69:82102 CA
 TITLE: Ground states of conjugated molecules. X. Fluorine-19 N.M.R. chemical shifts in aryl fluorides
 AUTHOR(S): Dewar, Michael J. S.; Kelemen, Jozsef
 CORPORATE SOURCE: Univ. of Texas, Austin, TX, USA
 SOURCE: Journal of Chemical Physics (1968), 49(2), 499-508
 CODEN: JCPSA6; ISSN: 0021-9606
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The procedures developed in previous papers of this series have been extended to aromatic fluorides, by using ^{19}F N.M.R. chem. shifts as a guide to the selection of parameters for F. Attempts to correlate chem. shifts with the local .pi.-electron d. on F proved unsatisfactory, the correlation depending on the no. of atoms ortho to F that carry p or .pi. electrons. Similar results followed for charge ds. calcd. by a recently developed semiempirical self-consistent field M.O. treatment in which all the valence electrons are included. Anal. of the Karplus-Das-Prosser-Goodman treatment of chem. shifts suggested that this "ortho effect" arose from neglected long-range interactions. A treatment including these was developed and shown to account well for the ^{19}F chem. shifts of nearly 100 aryl fluorides.
 IT 13180-38-6
 RL: PRP (Properties)
 (nuclear magnetic resonance of, electron configuration in relation to)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



IT 13180-38-6 13323-14-5
 RL: PRP (Properties)
 (nuclear magnetic resonance of, electron configuration in relation to)

10/607,220

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FILE 'REGISTRY' ENTERED AT 15:52:20 ON 02 JUN 2004

L1 STRUCTURE UPLOADED

L2 2 S L1 SAM

L3 39 S L1 FULL

FILE 'CA' ENTERED AT 15:52:47 ON 02 JUN 2004

L4 40 S L3

L5 22 S L3/PREP

L6 18 S L4 NOT L5

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---Logging off of STN---

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Executing the logoff script...

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STN INTERNATIONAL LOGOFF AT 15:53:57 ON 02 JUN 2004

L5 ANSWER 1 OF 5 CA COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 140:253457 CA

TITLE: Quinolyl propyl piperidine derivatives, the preparation thereof and compositions containing same, useful as antimicrobials

INVENTOR(S): Bacque, Eric; Bigot, Antony; El Ahmad, Youssef; Malleron, Jean Luc; Mignani, Serge; Ronan, Baptiste; Tabart, Michel; Viviani, Fabrice

PATENT ASSIGNEE(S): Aventis Pharma SA, Fr.

SOURCE: Fr. Demande, 96 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2844268	A1	20040312	FR 2002-11213	20020911
WO 2004024713	A1	20040325	WO 2003-FR2687	20030910
W: AE, AG, AL, AU, BA, BB, BR, BZ, CA, CN, CO, CR, CU, DM, DZ, EC, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NI, NO, NZ, OM, PG, PH, PL, RO, SC, SG, SY, TN, TT, UA, UZ, VC, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004082610	A1	20040429	US 2003-659095	20030910
PRIORITY APPLN. INFO.:			FR 2002-11213	A 20020911
OTHER SOURCE(S):		MARPAT 140:253457		

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB New 4-[3-(Quinol-4-yl)propyl]piperidine derivs. I are disclosed [wherein R1a = H, halo, OH, NH₂, alkylamino, dialkylamino, hydroxyamino, alkoxyamino, or alkylalkoxyamino; R1b = H, or R1aR1b = oxo; R2 = COOH, CH₂CO₂H, CH₂OH; R3 = C1-6 alkyl substituted by: (un)substituted SPh [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF₃, CF₃O, CO₂H, alkyloxycarbonyl, cyano, or NH₂], by 3- to 7-membered cycloalkylthio, or by 5- to 6-membered arom. heterocyclylthio comprising 1-4 N/O/S atoms and optionally substituted by halo, OH, alkyl, alkoxy, CF₃, CF₃O, COOH, alkyloxycarbonyl, cyano, or NH₂; or R3 = propargyl substituted by: Ph [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF₃, CF₃O, CO₂H, alkyloxycarbonyl, cyano, or NH₂], by cycloalkyl contg. 3-7 members, or by 5- to 6-membered arom. heterocyclyl with 1-4 N/O/S atoms [and (un)substituted by halo, OH, alkyl, alkoxy, CF₃, CF₃O, COOH, alkyloxycarbonyl, cyano, or NH₂]; R4 = C1-6 alkyl, alkenyl-CH₂, or alkynyl-CH₂ (alkenyls or alkynyls comprise 2-6 C atoms), cycloalkyl, or cycloalkylalkyl (cycloalkyls comprises 3-8 C atoms); including various isomers, enantiomeric and diastereoisomeric forms, mixts. and salts thereof]. The novel derivs. are particularly interesting as antimicrobial agents. Two synthetic examples are given. For example, II was prepd. by alkylation of III.bul.HCl (prepn. given) with

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2-(bromoethylsulfanyl)thiophene, followed by basic hydrolysis. In vivo, compds. I were active against exptl. infections of mice by Staphylococcus aureus IP 8203 at 12-150 mg/kg s.c., and at 26-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c.

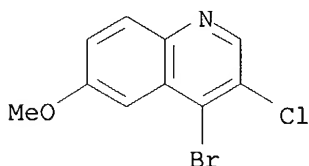
IT 426842-71-9, 4-Bromo-3-chloro-6-methoxyquinoline

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of quinolylpropyl piperidines as antimicrobial agents)

RN 426842-71-9 CA

CN Quinoline, 4-bromo-3-chloro-6-methoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 5 CA COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 140:235614 CA

TITLE: Quinolyl propyl piperidine derivatives, the preparation thereof and compositions containing same, useful as antimicrobials

INVENTOR(S): Bacque, Eric; Bigot, Antony; El Ahmad, Youssef; Malleron, Jean Luc; Mignani, Serge; Ronan, Baptiste; Tabart, Michel; Viviani, Fabrice

PATENT ASSIGNEE(S): Aventis Pharma SA, Fr.

SOURCE: Fr. Demande, 66 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2844270	A1	20040312	FR 2002-11212	20020911
WO 2004024712	A1	20040325	WO 2003-FR2686	20030910
W:	AE, AG, AL, AU, BA, BB, BR, BZ, CA, CN, CO, CR, CU, DM, DZ, EC, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NI, NO, NZ, OM, PG, PH, PL, RO, SC, SG, SY, TN, TT, UA, UZ, VC, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

US 2004087619 A1 20040506 US 2003-659164 20030910

PRIORITY APPLN. INFO.: FR 2002-11212 A 20020911

OTHER SOURCE(S): MARPAT 140:235614

GI

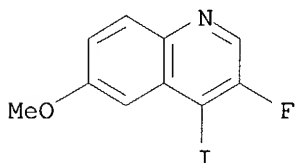
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB New 4-[3-(Quinol-4-yl)propyl]piperidine derivs. I are disclosed [wherein R1 = H or F; R2 = COOH, CH2CO2H, CH2OH; R3 = C1-6 alkyl substituted by: (un)substituted SPh [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by 3- to 7-membered cycloalkylthio, or by 5- to 6-membered arom. heterocyclylthio comprising 1-4 N/O/S atoms and optionally substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2; or R3 = propargyl substituted by: Ph [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by cycloalkyl contg. 3 -7 members, or by 5- to 6-membered arom. heterocyclyl with 1-4 N/O/S atoms [and (un)substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2]; R4 = C1-6 alkyl, alkenyl-CH2, or alkynyl-CH2 (alkenyls or alkynyls comprise 2-6 C atoms), cycloalkyl, or cycloalkylalkyl (cycloalkyls comprises 3-8 C atoms); including enantiomeric and diastereoisomeric forms, mixts. thereof, and salts thereof]. The novel derivs. are particularly interesting as antimicrobial agents. Five synthetic examples are given. For example, II was prepd. by N-alkylation of III (prepn. given) with 2-[(2-bromoethyl)sulfanyl]-1,4-difluorobenzene, followed by acidic hydrolysis. Compds. I were active against exptl. infections of mice by Staphylococcus aureus IP 8203 at 12-150 mg/kg s.c., and at 26-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c. (2 administrations).

IT 426842-84-4, 4-Iodo-3-fluoro-6-methoxyquinoline
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. of quinolylpropylpiperidines as antimicrobials)

RN 426842-84-4 CA

CN Quinoline, 3-fluoro-4-iodo-6-methoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 5 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 139:164798 CA
 TITLE: Preparation of aminopiperidine derivatives for treatment of bacterial infections
 INVENTOR(S): Miller, William Henry; Pearson, Neil David; Pendrak, Israil; Seefeld, Mark Andrew
 PATENT ASSIGNEE(S): Glaxo Group Limited, UK; Daines, Robert A
 SOURCE: PCT Int. Appl., 96 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003064421	A1	20030807	WO 2003-EP823	20030127
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,				

GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
 PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
 UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD,
 RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
 CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,
 NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW,
 ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

GB 2002-2026

A 20020129

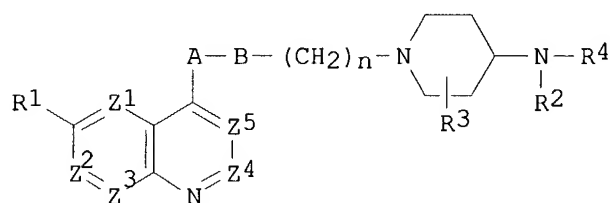
GB 2002-29824

A 20021220

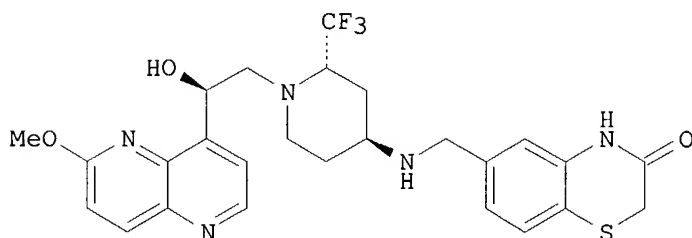
OTHER SOURCE(S):

MARPAT 139:164798

GI



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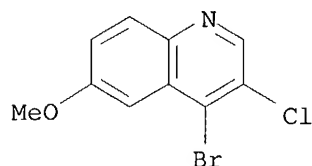


II

- AB Title compds. I [one of Z1-5 = N, one = CR1a and the remainder = CH or one of Z1-5 = CR1a and the remainder = CH; R1-1a = H, OH, alkoxy, amino, etc.; R2 = H, alkyl, alkenyl; R3 = CF3, 2-oxo, etc.; R4 = UR5; U = CO, SO2, CH2; R5 = bicyclic, heterocyclic ring system A; n = 0-1; AB = amido, alkylacyl, aminosulfonyl, etc.] are prepd. For instance, bromomethyl (6-methoxy[1,5]naphthyridin-4-yl)ketone (prepn. given) is reduced (PhMe, (+)-DIPCl) to give the (R)-alc., converted to the oxirane (MeOH, K2CO3) and used to alkylate [(2S,4S)-2-(trifluoromethyl)piperidin-4-yl]carbamic acid tert-Bu ester (prepn. given) and deprotected to give (1R)-2-[(2S,4S)-4-amino-2-(trifluoromethyl)piperidin-1-yl]-1-(6-methoxy[1,5]naphthyridin-4-yl)ethanol. This amine is alkylated with 3-oxo-3,4-dihydro-2H-benzo[1,4]thiazine-6-carboxaldehyde (prepn. given) (EtOH, NaBH4) to give II. Selected examples have MICs .ltoreq. 2 .mu.g/mL vs., e.g., *S. epidermidis* CL7, *S. aureus* WCUH29, etc.
- IT 426842-71-9P, 4-Bromo-3-chloro-6-methoxyquinoline
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of aminopiperidine derivs. for treatment of bacterial

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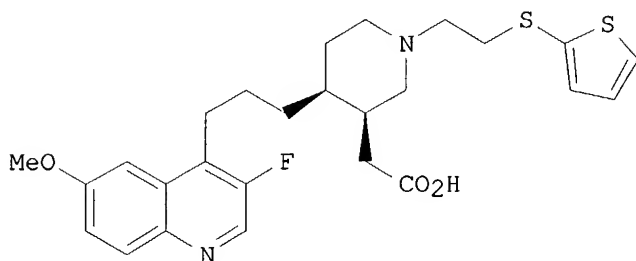
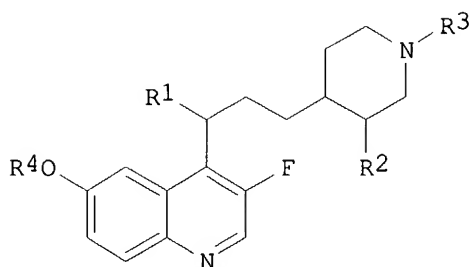
infections)
RN 426842-71-9 CA
CN Quinoline, 4-bromo-3-chloro-6-methoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 5 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 137:232568 CA
TITLE: Quinolyl propyl piperidine derivatives, the preparation thereof and compositions containing same, useful as antimicrobials
INVENTOR(S): Bacque, Eric; Mignani, Serge; Malleron, Jean-Luc; Tabart, Michel; Evers, Michel; Viviani, Fabrice; El-Ahmad, Youssef; Mutti, Stephane; Daubie, Christophe
PATENT ASSIGNEE(S): Aventis Pharma S.A., Fr.
SOURCE: PCT Int. Appl., 71 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002072572	A1	20020919	WO 2002-FR851	20020311
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
FR 2822154	A1	20020920	FR 2001-3374	20010313
EP 1370550	A1	20031217	EP 2002-722329	20020311
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
US 2002177606	A1	20021128	US 2002-96482	20020313
US 6602884	B2	20030805		
US 2003171369	A1	20030911	US 2003-387479	20030314
PRIORITY APPLN. INFO.:			FR 2001-3374	A 20010313
			US 2001-281407P	P 20010405
			WO 2002-FR851	W 20020311
			US 2002-96482	A3 20020313
OTHER SOURCE(S):		MARPAT 137:232568		
GI				



AB New 4-[3-(Quinol-4-yl)propyl]piperidine derivs. I are disclosed [wherein R1 = H, halo, OH, NH2, alkylamino, dialkylamino, hydroxyamino, alkoxyamino, or alkylalkoxyamino; R2 = COOH, CH2CO2H, CH2OH; R3 = C1-6 alkyl substituted by: (un)substituted SPh [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by 3- to 7-membered cycloalkylthio, or by 5- to 6-membered arom. heterocyclylthio comprising 1-4 N/O/S atoms and optionally substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2; or R3 = propargyl substituted by: Ph [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by cycloalkyl contg. 3-7 members, or by 5- to 6-membered arom. heterocyclyl with 1-4 N/O/S atoms [and (un)substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2]; R4 = C1-6 alkyl, alkenyl-CH2, or alkynyl-CH2- (alkenyls or alkynyls comprise 2-6 C atoms), cycloalkyl, or cycloalkylalkyl (cycloalkyls comprises 3-8 C atoms); including diastereoisomeric forms, mixts. thereof, cis or trans forms, and salts thereof]. The novel derivs. are particularly interesting as antimicrobial agents. Ten synthetic examples are given. For instance, Wittig reaction of 4(RS)-4-allyl-1-(benzyloxycarbonyl)piperidin-3-one with Ph3P:CHCO2Me gave a Z-isomeric exocyclic olefin, which underwent hydroboration at allyl and Pd-catalyzed coupling with 4-iodo-3-fluoro-6-methoxyquinoline, followed by hydrogenation of the olefin with concomitant N-deprotection, N-alkylation with 2-(2-bromoethylthio)thiophene, and sapon. of the Me ester, to give the racemic title compd. II.2HCl. Compds. I were active against exptl. infections of mice by *Staphylococcus aureus* IP 8203 at 12-150 mg/kg s.c., and at 26-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c. (2 administrations).

IT **426842-84-4**, 4-Iodo-3-fluoro-6-methoxyquinoline

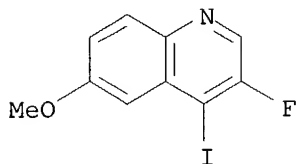
RL: RCT (Reactant); RACT (Reactant or reagent)

(precursor; prepn. of (quinolylpropyl)piperidine derivs. as antimicrobials)

RN 426842-84-4 CA

10/607,220

CN Quinoline, 3-fluoro-4-iodo-6-methoxy- (9CI) (CA INDEX NAME)



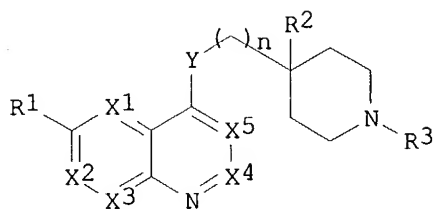
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 5 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 136:386033 CA
TITLE: Heterocyclalkyl piperidine derivatives, particularly 4-[3-(quinolin-4-yl)propyl]piperidine-4-carboxylic acids, their preparation and compositions containing same, for use as antibacterials.
INVENTOR(S): Bacque, Eric; Carry, Jean-Christophe; El-Ahmad, Youssef; Evers, Michel; Hubert, Philippe; Malleron, Jean-Luc; Mignani, Serge; Pantel, Guy; Tabart, Michel; Viviani, Fabrice
PATENT ASSIGNEE(S): Aventis Pharma S.A., Fr.
SOURCE: PCT Int. Appl., 362 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

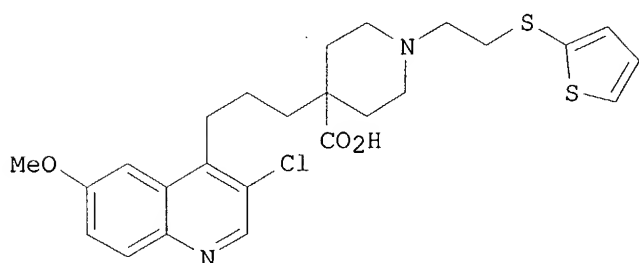
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002040474	A2	20020523	WO 2001-FR3559	20011114
WO 2002040474	A3	20021031		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
FR 2816618	A1	20020517	FR 2000-14738	20001115
FR 2816618	B1	20021227		
AU 2002018365	A5	20020527	AU 2002-18365	20011114
US 2002111492	A1	20020815	US 2001-987386	20011114
US 6603005	B2	20030805		
EE 200300207	A	20030815	EE 2003-207	20011114
EP 1337529	A2	20030827	EP 2001-996538	20011114
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
BR 2001015312	A	20030923	BR 2001-15312	20011114
JP 2004514661	T2	20040520	JP 2002-543484	20011114
NO 2003002187	A	20030626	NO 2003-2187	20030514
PRIORITY APPLN. INFO.:			FR 2000-14738	A 20001115
			US 2000-255145P	P 20001214
			WO 2001-FR3559	W 20011114

OTHER SOURCE(S):
GI

MARPAT 136:386033



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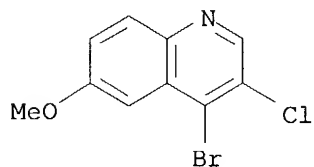
- AB The invention concerns heterocyclylalkyl piperidine derivs. I, including their enantiomeric or diastereoisomeric forms, or mixts. thereof, and/or their syn or anti forms, or mixts. thereof, and their salts [wherein X1, X2, X3, X4, and X5 = C(R'1), C(R'2), C(R'3), C(R'4), C(R'5), or one of X-groups (at most) = N; R1, R'1, R'2, R'3, R'4, R'5 = H, halo, alkyl, cycloalkyl, Ph, PhS, OH, heterocyclyl, cyano, CO2H, alkoxy carbonyl, (un)substituted NH2, etc.; R2 = CO2H, alkyloxy carbonyl, cycloalkyloxy carbonyl, cyano, CONRaRb, CH2OH, substituted alkyl, CF2-Rc, C(CH3)2-Rc, CORc, CH(OH)-Rc, C(cycloalkyl)-Rc, or CH:CH-Rc; Ra, Rb = H, alkyl, cycloalkyl, Ph, heterocyclyl; or NRaRb = (un)substituted 5- or 6-membered heterocycle; Rc = CO2H, alkoxy carbonyl, cycloalkoxy carbonyl, CONRaRb; R3 = Ph, heterocyclyl, various substituted alkyls; Y = CH(Re), CF2, C(:NOH), alkyloxyiminomethylene, cycloalkyloxyiminomethylene, or C3-6 cycloalkylidene; Re = H, F, OH, alkoxy, cycloalkoxy, CO2H, alkoxy carbonyl, NRaRb, CONRaRb; and n = 0-4; wherein the radicals or Ph or heterocyclyl portions mentioned above can optionally be substituted]. Approx. 60 compds. were prep'd., 5 were specifically claimed, and many more names were listed. For instance, Pd-complex-catalyzed coupling of 4-allyl-4-Cbz-1-BOC-piperidine with 4-bromo-3-chloro-6-methoxyquinoline (preps. of both compds. given), followed by removal of the BOC group with CF3CO2H, N-alkylation with 2-[(2-bromoethyl)thio]thiophene, and hydrolysis of the benzyl ester (Cbz) in aq. HCl, gave title compd. II as the di-HCl salt. I were active against both gram-pos. and gram-neg. bacteria. I were active against exptl. infection of mice with Staphylococcus aureus IP8203 at 18-150 mg/kg s.c., or 20-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c. (2 administrations).
- IT **426842-71-9P**, 4-Bromo-3-chloro-6-methoxyquinoline
426842-84-4P, 4-Iodo-3-fluoro-6-methoxyquinoline
426842-86-6P, 4-Chloro-3-fluoro-6-methoxyquinoline
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

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(intermediate; prepn. of quinolinylpropylpiperidinecarboxylic acids as
antibacterials.)

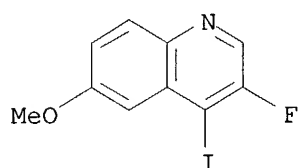
RN 426842-71-9 CA

CN Quinoline, 4-bromo-3-chloro-6-methoxy- (9CI) (CA INDEX NAME)



RN 426842-84-4 CA

CN Quinoline, 3-fluoro-4-iodo-6-methoxy- (9CI) (CA INDEX NAME)



RN 426842-86-6 CA

CN Quinoline, 4-chloro-3-fluoro-6-methoxy- (9CI) (CA INDEX NAME)

